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ANALYSIS OF THE TEMPERATURE DEPENDENCE OF RESISTIVITY IN N-TYPE--ETC(U)

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ANALYSIS OF THE TEMPERATURE DEPENDENCE OF RESISTIVITY IN N-TYPE SILICON

The BDM Corporation
P.O. Box 9274
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PREFACE

This report was prepared by The BDM Corporation, 1801 Randolph Road, S.E., Albuquerque, New Mexico 87106, for Defense Nuclear Agency, Washington, D.C. 20305, to supplement work done under contract DNA 001-79-C-0138. It consists of an analytical development of the observed temperature dependence of resistivity in n-type silicon. This is accomplished by considering the temperature dependence of each physical parameter contributing to resistivity in various doping ranges. Knowledge of this thermal behavior of resistivity is critical to semiconductor device operation under thermal stress. The BDM author was Ms. M. Glaubenslee.

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CHAPTER I INTRODUCTION

This paper attempts to explain some theoretical basis for the observed temperature dependence of resistivity, ρ , in n-type silicon. This dependence is known to be influenced by doping density and these effects can be seen in figure I-1. The aim of this discussion is the explanation of this graph in both a general qualitative sense and a more explicit deliniation of the functional dependence of $\rho(T)$. This functional dependence is a composite of the analytical representations of the various physical parameters contributing to resistivity. These parameters and the physical phenomena they describe will be discussed as they relate to resistivity in n-type silicon.

The results of this more or less theoretical treatment of resistivity are then compared to empirical graphs and show remarkable agreement. Such a reliable theoretical basis for the thermal behavior of resistivity is critical to all thermal processes affecting semiconductor device operation.

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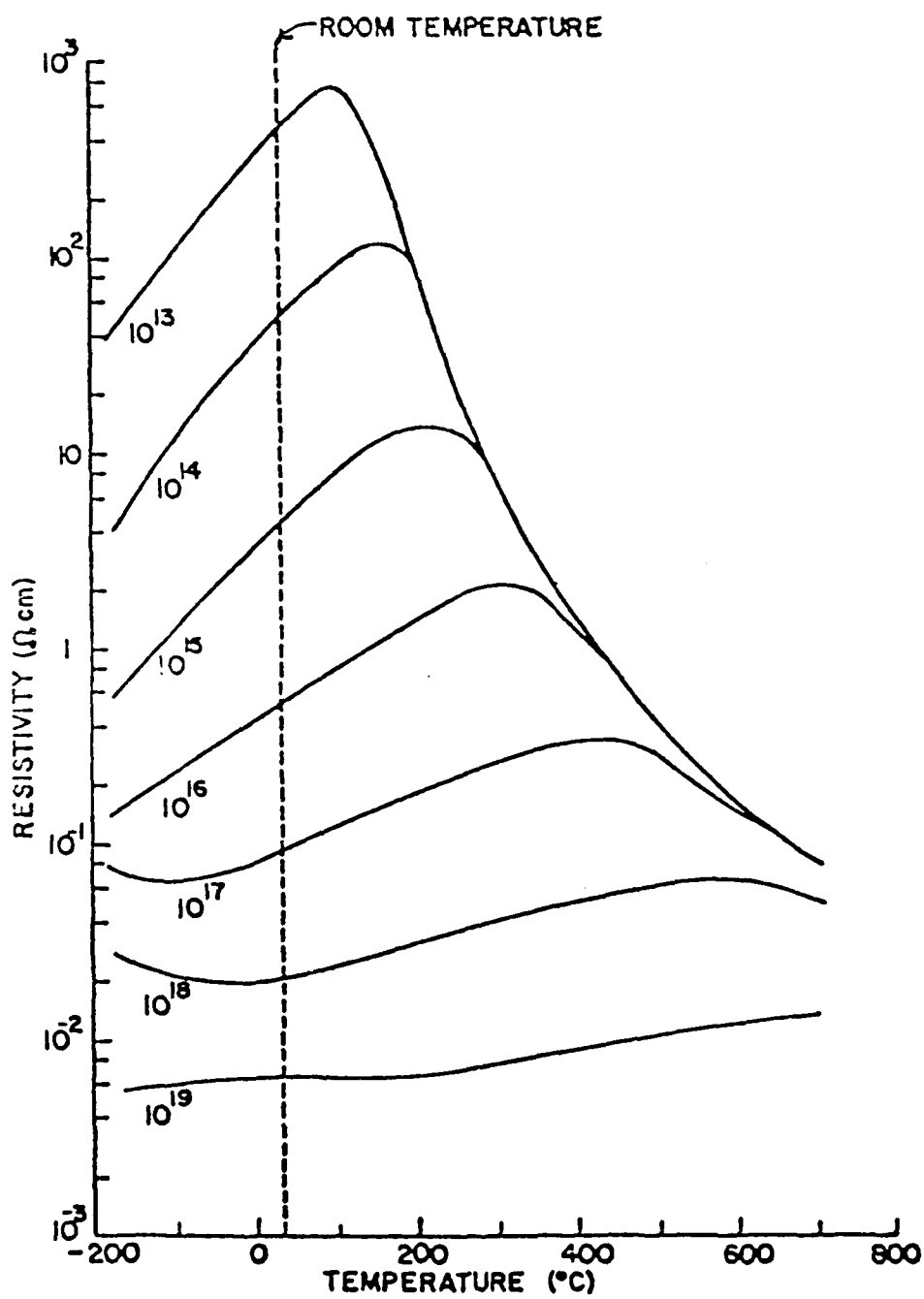


Figure I-1. Silicon Resistivity Versus Temperature

CHAPTER II BACKGROUND

The current density transported by electrons and holes in any semi-conductor is given by:

$$\vec{I}_n = ne\mu_n\vec{E}$$

$$\vec{I}_p = pe\mu_p\vec{E}$$

where e = charge of electron

n = electron density

p = hole density

μ_n = electron mobility

μ_p = hole mobility

\vec{E} = electrical field intensity.

Thus, the total electrical current density, \vec{I} , may be given as:

$$\vec{I} = e(n\mu_n + p\mu_p)\vec{E} = \sigma\vec{E}$$

where the electrical conductivity, σ , is expressed as:

$$\sigma = e(n\mu_n + p\mu_p)$$

and the resistivity is defined as:

$$\rho = \frac{1}{\sigma} = \frac{1}{e(n\mu_n + p\mu_p)} \quad (1)$$

In this expression n and p are the actual instantaneous values of electron and hole concentration. n , p , μ_n , μ_p are functions of temperature and thereby determine the temperature dependence of ρ . It is further

assumed in this expression that the charges trapped by donors and acceptors are immobile and that n , p , μ_n , μ_p are independent of \vec{E} . This is true only for low \vec{E} -field intensities, where no gradients of carrier density are considered that may give rise to diffusion currents.

If only the equilibrium state is considered, then:

$$\rho_0 = \frac{1}{e(n_0 \mu_n + p_0 \mu_p)}$$

where n_0 and p_0 are the equilibrium carrier densities.

CHAPTER III QUALITATIVE ASPECTS OF THE DEPENDENCE OF ρ ON TEMPERATURE

A. INTRINSIC SEMICONDUCTORS

Semiconductors can behave either intrinsically or nonintrinsically. An intrinsic semiconductor is a pure or undoped semiconductor with equal carrier concentrations. For this case the temperature dependence of resistivity can be given in terms of the intrinsic carrier concentration, n_i , where:

$$n_i = n_o = p_o = 2 \left(\frac{2\pi(M_p^* M_n^*)^{1/2} k T}{h^2} \right)^{3/2} \exp \left(\frac{-E_g}{2kT} \right)$$

M_p^* = hole effective mass

M_n^* = electron effective mass

k = Boltzmann constant

T = absolute temperature

h = Plank's constant

E_g = gap energy.

Therefore,

$$\rho_o = \frac{1}{en_i(\mu_n + \mu_p)}$$

The temperature dependence of μ will later be shown to be predominantly a $T^{-3/2}$ dependence. This will generally cancel the $T^{3/2}$ dependence of n_i . Therefore a plot of ρ_o versus $1/T$ in an essentially intrinsic semiconductor should be approximately linear.

B. NON-INTRINSIC SEMICONDUCTORS

A non-intrinsic semiconductor depends on the addition of impurity atoms to provide additional donor and/or acceptor states and thereby enhance its conduction properties. The effect of such dopant densities on resistivity can be explained by considering their contribution to the carrier density in a semiconductor. This can be seen by considering charge neutrality:

$$n + N_a^- = p + N_d^+$$

where N_a^- = charge density due to occupied acceptor states

N_d^+ = charge density due to ionized (or unoccupied) donor states.

At temperatures above room temperature all typical donors and acceptors in silicon are completely ionized; therefore,

$N_a^- = N_a$ = acceptor atom dopant density

$N_d^+ = N_d$ = donor atom dopant density.

If such total ionization is assumed for an n-type ($N_d > N_a$) semiconductor, then substitution for n or p (from $np = n_i^2$) makes the charge neutrality equation quadratic in n or p. Solving this equation gives expressions for n and p in terms of the donor and/or acceptor densities.

$$n \approx \frac{N_d - N_a}{2} + \sqrt{\left(\frac{N_d - N_a}{2}\right)^2 + n_i^2} \quad (2)$$

$$p \approx -\frac{N_d - N_a}{2} + \sqrt{\left(\frac{N_d - N_a}{2}\right)^2 + n_i^2} \quad (3)$$

Now these expressions can be substituted into equation (1) to give the resistivity in terms of μ_n , μ_p and N_a , and N_d .

$$\rho = \frac{1}{e \left\{ \left(\frac{N_d - N_a}{2} + \sqrt{\frac{(N_d - N_a)^2}{4} + n_i^2} \right) \mu_n + \left(-\frac{N_d - N_a}{2} + \sqrt{\frac{(N_d - N_a)^2}{4} + n_i^2} \right) \mu_p \right\}} \quad (4)$$

1. Higher Temperature Region

It can be seen in figure III-1 that n_i increases rapidly with temperature; therefore, for sufficiently high temperatures $n_i \gg N_d - N_a$, which is just some constant value. Employing this condition then reduces equations (2) and (3) to:

$$n \approx n_i + \frac{N_d - N_a}{2}$$

$$p \approx n_i - \frac{N_d - N_a}{2}$$

When these expressions are substituted into equation (4) the expression for ρ becomes:

$$\rho = \frac{1}{en_i(\mu_n + \mu_p)}$$

which is the intrinsic result. In general, all semiconductors behave intrinsically at sufficiently high temperature. This intrinsic carrier behavior is seen in figure III-2 for an n-type semiconductor.

2. Lower Temperature Region

Again, due to the strong temperature dependence of n_i , for a sufficiently low temperature, $n_i \ll N_d - N_a$. In this region equations (2) and (3) reduce to:

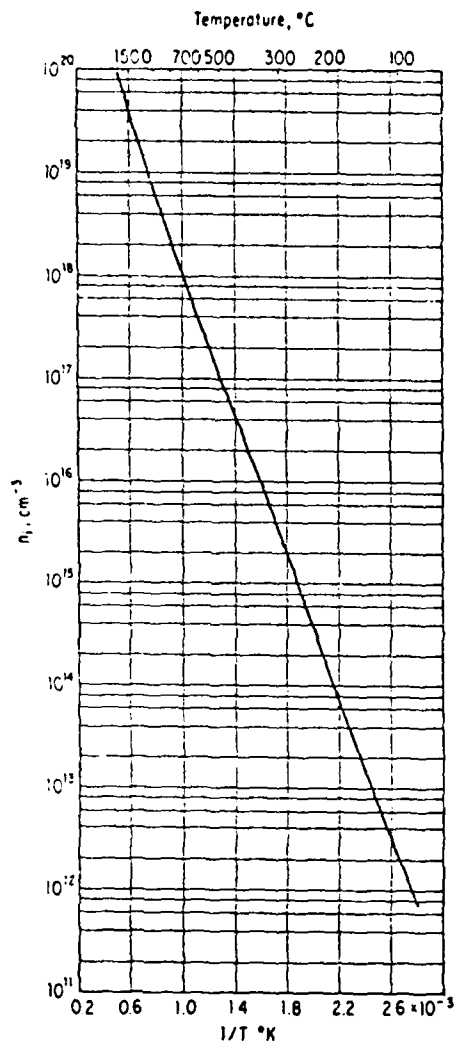


Figure III-1. Intrinsic Carrier Concentration n_i Versus Reciprocal Temperature

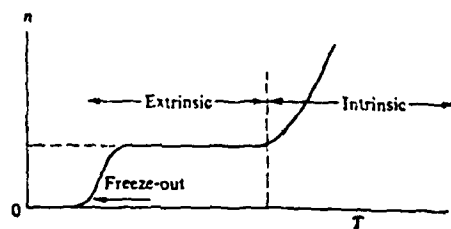


Figure III-2. Variation of Electron Concentration n with Temperature in an n-Type Semiconductor

$$n \approx N_d - N_a$$

$$p \approx 0$$

for an n-type ($N_d > N_a$) semiconductor, see figure III-2.

The resistivity then becomes just:

$$\rho = \frac{1}{e\mu_n(N_d - N_a)}$$

Here the temperature dependence is merely that of μ_n (which will be discussed later in detail). This dependence is, however, primarily a $T^{-3/2}$ dominated function.

As the temperature is progressively lowered, the thermal energy becomes too small to cause sufficient excitations to keep electrons in the conduction band. At these low temperatures free electrons and holes are "frozen out" of the conduction band back into the donor and acceptor states (see figure III-2). Thus, the carrier concentration, $N_d - N_a$, is depleted, resulting in an increased resistivity.

3. Transition Region

The transition between the two temperature regions where $n_i \ll N_d - N_a$ and $n_i \gg N_d - N_a$ occurs where $n_i \approx N_d - N_a$. As seen in figure III-1, this transition temperature increases as n_i increases. Therefore, as the impurity density $N_d - N_a$ increases, the transition temperature also increases.

C. NONAPPLICABILITY EQUATION (1)

1. Very High Impurity Densities

At high impurity densities the wave functions of electrons on neighboring donor atoms or of holes on neighboring acceptor atoms will overlap significantly. This acts to broaden the donor or acceptor level into a narrow energy band. Since there are more states than electrons

(or holes) in this band, the possibility of "impurity band conductivity" exists. We have initially assumed in equation (1) that the charges trapped by the donors and acceptors are immobile. However, at these high impurity concentrations, a trapped charge may hop from one impurity atom to another causing current overflow.

2. High \vec{E} Field Effects

Equation (1) assumes the mobilities and carrier concentrations to be independent of the applied electric field. For high fields this is not so. The number of carriers may remain essentially constant but their mobility decreases appreciably. Figure III-3 shows the dependence of mobility on field strength for n-type silicon. At high enough field intensities ($> 10^5$ V/cm) carriers can obtain velocities sufficient to form new carriers upon collision.

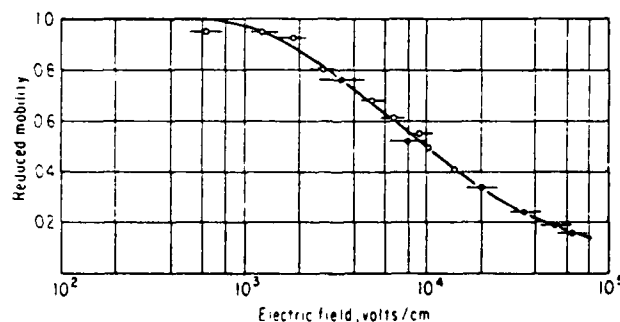


Figure III-3. Variation of Reduced Mobility with Electric Field Applied to 70 ohm-cm Silicon Along the $\langle 111 \rangle$ Direction. Carrier Concentration Assumed Constant.

CHAPTER IV

QUANTITATIVE ASPECTS OF THE DEPENDENCE OF ρ ON TEMPERATURE

So far only the qualitative features of the temperature dependence of resistivity in semiconductors have been considered. In this section a quantitative approach to the various parametric contributions to the temperature dependence of resistivity will be considered.

Since resistivity is given by the expression:

$$\rho = \frac{1}{e(n\mu_n + p\mu_p)}$$

the parameters that determine its functional dependence are n , p , μ_n , and μ_p .

Now the temperature dependence of the carrier concentrations are fairly straightforward and are given by:

$$n = 2 \left(\frac{2\pi m_e kT}{h^2} \right)^{3/2} \exp \left(-\frac{E_c - E_f}{kt} \right) \approx \frac{N_d - N_a}{2} + \sqrt{\left(\frac{N_d - N_a}{2} \right)^2 + n_i^2}$$

$$p = 2 \left(\frac{2\pi m_p kT}{h^2} \right)^{3/2} \exp \left(-\frac{E_f - E_v}{kt} \right) \approx -\frac{N_d - N_a}{2} + \sqrt{\left(\frac{N_d - N_a}{2} \right)^2 + n_i^2}$$

where E_c = energy of conduction band

E_v = energy of valence band

E_f = Fermi energy.

However, the temperature dependence of the mobilities of these carriers is not deduced in so straightforward a manner. This has to do with the fact that mobility is a measure of the swiftness with which a carrier is propagated through the semiconductor. This swiftness in turn depends on the frequency of collisions the carrier encounters on its way. Such collisions are the result of various scattering mechanisms available to the carrier within the solid, which include:

- (1) Lattice scattering
- (2) Ionized impurity scattering
- (3) Neutral impurity scattering
- (4) Electron-electron scattering.

These scattering phenomena affect the carrier lifetime (or relaxation time), τ , between collisions, and thereby determine carrier mobility:

$$\mu = \frac{e\tau}{m}$$

Thus, the temperature dependence of mobility is determined by the temperature dependence of the carrier relaxation time due to a variety of scattering possibilities.

Of these the most significant for nonpolar semiconductors, such as silicon, are lattice scattering and scattering due to ionized impurities.

1. Lattice Scattering

Mobility due to lattice scattering was analyzed extensively by Norton, et. al., (2) for n-type silicon over a temperature range of 100 to 500°K. Their calculations include contributions from both intravalley acoustical phonon scattering and intervalley optical phonon scattering, as well as anisotropic considerations. The processes of intervalley and intervalley scattering must be considered in a semiconductor having several equivalent conduction band minima, where carriers can be scattered from one minima to another as well as scattered within the same band minima. Due to the higher energies involved in transition, intervalley scattering becomes important only at temperatures high enough so that an appreciable number of suitable phonons are excited.

Their average lattice scattering mobility expression is given by:

$$\mu_L = \frac{1}{3}e \left(\frac{\langle \tau_{||} \rangle}{M_{||}^*} + 2 \frac{\langle \tau_{\perp} \rangle}{M_{\perp}^*} \right)$$

where $\tau_{||}$ and τ_{\perp} refer to relaxation times in the longitudinal and two mutually perpendicular transverse directions. These are given by:

$$\frac{1}{\tau_{L\perp}} = \frac{T^{3/2} x^{1/2}}{\tau_0} \left(1 + \sum_i \left\{ \omega_i \left(\frac{\theta_i}{T} \right) \left[n_i \left(1 + \frac{\theta_i}{Tx} \right)^{1/2} + (n_i + 1) \left(1 - \frac{\theta_i}{Tx} \right)^{1/2} \right] \right\} \right)$$

θ_i = temperature of the i th intervalley phonon

$n_i = [\exp(\theta_i/T) - 1]^{-1}$

ω_i = the relative coupling strength of the electrons to the i th intervalley (adjusted to give best fit to observed data)

$x = E_g/kT$

$$\frac{1}{\tau_{L\parallel}} = \frac{1}{\tau_{L\perp}} + \frac{T^{3/2} x^{1/2}}{2\tau_0}$$

Each average is then computed using:

$$\langle T \rangle = \frac{4}{3\sqrt{\pi}} \int_0^{\infty} e^{-x} x^{3/2} \tau(x) dx$$

where $x = E_g/kT$, and the integral is numerically evaluated using Simpson's rule. Values of μ_L have been tabulated for temperatures in the range of 100° to 500°K for n-type silicon and are available in reference 1.

2. Ionized Impurity Scattering

For lightly doped n-type silicon the main contribution to the electron mobility comes from lattice scattering. However, as dopant density increases (or temperature decreases) the role of impurity scattering becomes more and more important. The most classic formula for ionized impurity scattering is the Brooks-Herring formula (6) which is derived assuming fixed scattering centers, spherical energy surfaces, and negligible electron-electron scattering contributions. The expressions in this derivation are given by:

$$\tau_I = \frac{(2M_n^*)^{1/2} \epsilon_s E^{3/2}}{\pi e^4 N_I G(b)} \times 10^{-6}$$

where ϵ_s = permittivity of Si ($11.7 \epsilon_0$)

E = electron energy

N_I = net ionized impurity density

$$G(b) = \ln(b+1) - \frac{b}{b+1}$$

where

$$b = \frac{24\pi M_n^* \epsilon_s (kT)^2}{e^2 h^2 n} \times 10^{-6}$$

and

$$n^i = n \times \left(2 - \frac{n}{N_D}\right) \quad \text{for } N_a = 0$$

The expression for τ_I gives the following result for ionized impurity scattering:

$$\mu_{I(BH)} = \frac{2^{7/2} \epsilon_s^2 (kT)^{3/2}}{\pi^{3/2} e^3 M_n^{*1/2} N_I G(b)} \times 10^{-2}$$

However, this expression neglects the effects of anisotropic scattering. Norton, et. al., (2) have made this adjustment to give:

$$\mu_I = \frac{7.3 \times 10^{17} T^{3/2}}{N_I G(b_g)}$$

where b_g makes the replacement of $M_l^* = 0.98 M_n$ in the expression for b .

3. Neutral Impurity Scattering

By considering neutral impurity scattering as a problem analogous to the scattering of slow electrons by hydrogen atoms, Sclar (3) has derived a temperature-dependent electron mobility expression given by:

$$\mu_N = 0.82\mu_{NE} \left[2/3 \left(\frac{kT}{E_N} \right)^{1/2} + 1/3 \left(\frac{E_N}{kT} \right)^{1/2} \right]$$

where

$$E_N = 1.136 \times 10^{-19} \left(\frac{M_n^*}{M_0} \right) \left(\frac{\epsilon_0}{\epsilon_s} \right) \quad (\text{binding energy})$$

$$\mu_{NE} = \frac{2\pi^3 e^3 M_n^*}{5 N_N \epsilon_s h^3} \times 10^{-2}$$

N_N = neutral donor density

Note $\mu_N \sim T^{1/2}$ for $kT > E_N$

4. Electron-Electron Scattering

The last contribution to electron mobility that has so far been neglected is that due to electron-electron (e-e) scattering.

Electron-electron scattering does not affect current density directly since it can alter the momentum distribution among electrons without altering the total momentum. Electron-electron scattering allows momentum to be transferred from those electrons which dissipate momentum less efficiently to those which dissipate it more efficiently; resulting in a greater overall rate of momentum transfer and a lower mobility.

On the basis of such an argument, the effect of e-e scattering mobility will depend on the electron energy, E . Thus, ionized impurity scattering relaxation time ($\sim E^{3/2}$) will be more strongly affected by e-e scattering than lattice scattering relaxation time ($\sim E^{-1/2}$). The effects of both scattering modes have been analyzed by Li, et. al., (1) and are given as follows:

- corrected ionized impurity mobility -

$$\mu_I' = (1 - e^{-n/N_I}) \cdot \mu_I$$

The effect of e-e scattering becomes more important on ionized impurity mobility as doping increases ($N_D > 2 \times 10^{16} \text{cm}^{-3}$).

- corrected lattice mobility -

$$\mu_L' = 0.88 \mu_L$$

5. Mobility Expressions Due To Combined Scattering Effects

Now that the necessary mobility expressions for the various scattering processes have been defined, their contributions must be combined in some suitable manner. The combined mobility due to both lattice and ionized impurity scattering contributions can be calculated according to a formula developed by Debye and Conwell (4). This formula is the result of an integrated average given by:

$$\mu_{LI} = \frac{e}{m} \frac{\langle v^2 \tau_{LI} \rangle}{\langle v^2 \rangle}$$

where

$$\frac{1}{\tau_{LI}} = \frac{1}{\tau_L} + \frac{1}{\tau_I}$$

The form of this integral can be evaluated in closed form only when the G(b) temperature dependence in τ_I is approximated by a suitable constant. When this is done the integral obtained is the so called "mixed scattering formula" given by:

$$\mu_{LI} = \mu_L \left[1 + X^2 \left\{ \text{Ci}(X) \cos X + \sin X \left(\text{Si}(X) - \frac{\pi}{2} \right) \right\} \right]$$

where $Ci(X)$ and $Si(X)$ are the cosine and sine integrals of X respectively. However, X is dependent on the degree of e-e scattering, which in turn depends on the dopant density.

For low donor densities ($N_D < 2 \times 10^{16} \text{ cm}^{-3}$), the effect of e-e scattering is negligible and X^2 is given by:

$$X^2 = 6\mu_L/\mu_I$$

In the intermediate dopant density range ($2 \times 10^{16} < N_D < 2 \times 10^{17} \text{ cm}^{-3}$), the effects of e-e scattering on μ_L and μ_I are gradual and not well defined. Therefore, theoretical mobility calculations for lattice and ionized impurity scattering in this range, are empirically fit to observed data by the use of so-called "mobility reduction factors." The ranges of these factors are given for both scattering processes in the mobility expressions:

$$\mu_L'' = ((1.013 \text{ to } 6.63) \times 10^{-19} \times N_D) \mu_L$$

$$\mu_I'' = ((1.04 \text{ to } 2.04) \times 10^{-18} \times N_D) \mu_I$$

In this range X'' is substituted into the mixed scattering formula where X'' is given by:

$$(X'')^2 = 6\mu_L''/\mu_I''$$

The effects of lattice scattering as well as ionized impurity scattering and e-e scattering have been considered in deriving the expression for μ_{LI} . If neutral impurity scattering is also included the electron mobility due to all the discussed scattering phenomena is given by:

$$\mu_n = \left(\mu_{LI}^{-1} + \mu_N^{-1} \right)^{-1}$$

6. Temperature Dependence of ρ

Recall for n-type silicon the carrier concentration is given by:

$$n = N_c \left(\exp \left(\frac{E_c - E_f}{kT} \right) + 0.27 \right)^{-1} \quad E_f < 1.3kT$$

where

$$N_c = 2 \left(\frac{2\pi M_d^* kT}{h^2} \right)^{3/2}$$

and M_d^* = density of states effective mass.

Using this and the final result of section IV.5, the expression for resistivity is given by:

$$\rho = \frac{1}{en\mu_n}$$

where e = charge of electron

n = given above

μ_n = given in section IV.5

ρ can now be calculated using these expressions and plotted as a function of T . This was done for a range of temperatures from 100 to 500°K for various dopant densities and the results are given in figure IV-1. These results correspond very well to experimental resistivity data as can be seen in figure IV-2. Thus, the functional dependence of ρ on T as determined by the parametric dependence of μ_n and n on T derived herein must be correct. That is, the temperature-dependent scattering modes discussed must be the principle phenomena determining electron mobility in an n-type semiconductor.

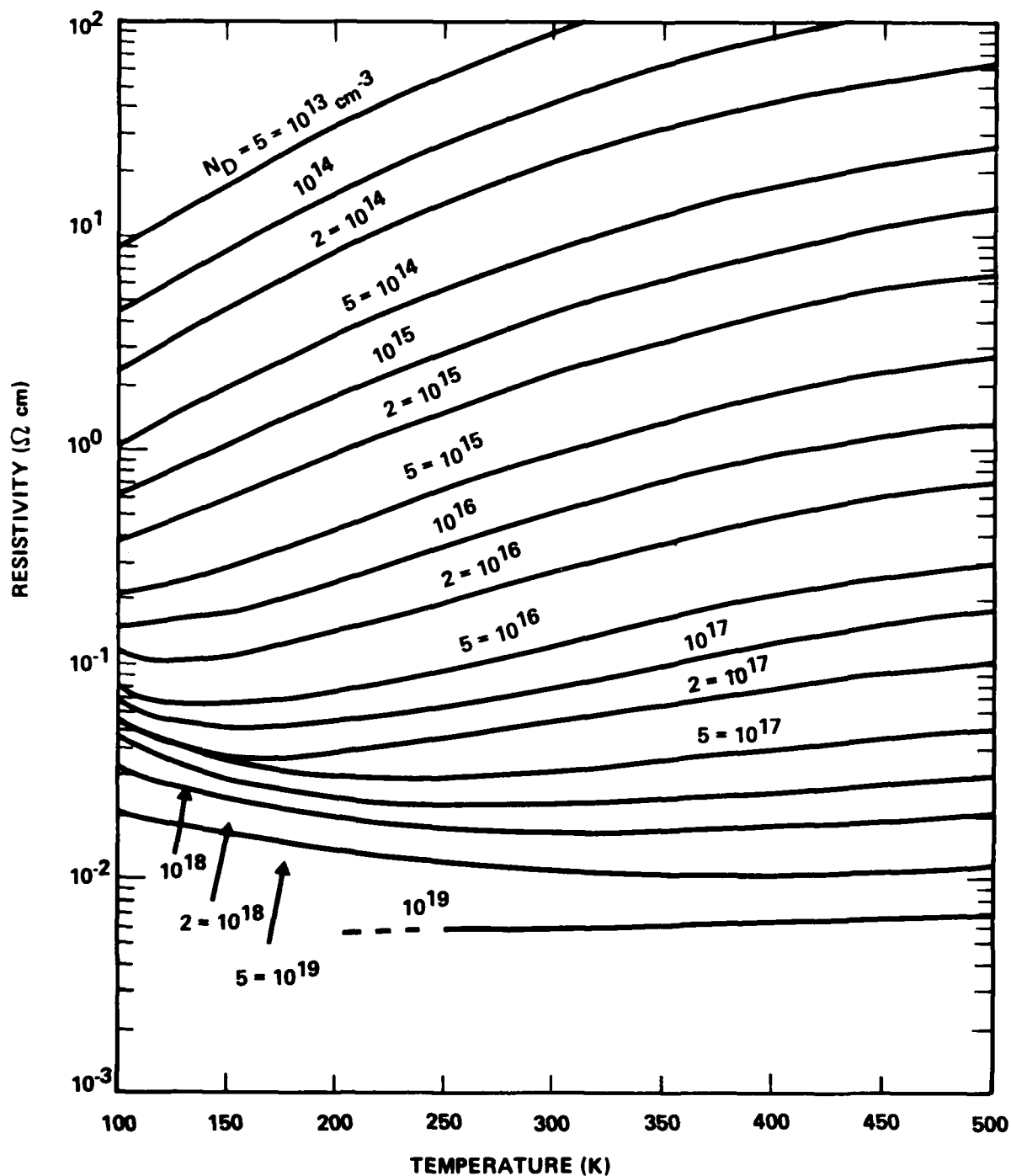


Figure IV-1. Theoretical Calculations of Resistivity Versus Temperature for n-Type Silicon for Dopant Densities from 5×10^{13} to 10^{19} cm^{-3}

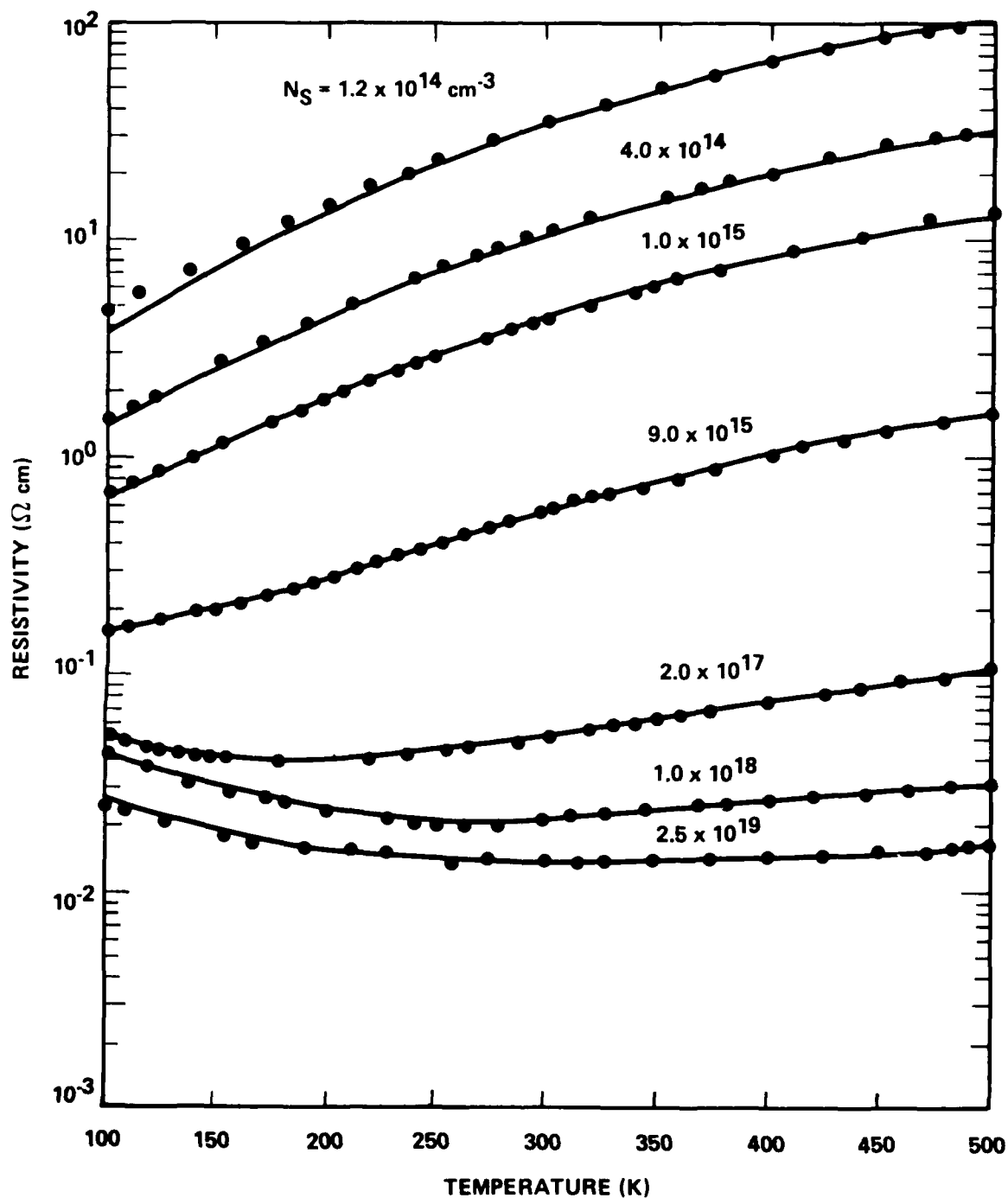


Figure IV-2. Resistivity Versus Temperature for Seven Phosphorus-Doped Silicon Samples. Solid Lines Are the Theoretical Calculation and Dots Are the Experimental Data.

In addition to this graphical dependence of ρ on T , table 1 summarizes the analytical dependence of ρ , n and μ for various dopant density ranges in n-type silicon.

TABLE 1. ANALYTICAL TEMPERATURE DEPENDENCE OF THE RESISTIVITY (ρ) OF n-TYPE SILICON FOR VARIOUS DOPING RANGES

ρ		$\rho = \frac{1}{en\mu_n}$		
n		$n = N_c \left(\exp \left(\frac{E_c - E_f}{kT} \right) + .27 \right)^{-1}$ where $N_c = 2 \left(\frac{2\pi m_d^* kT}{h^2} \right)^{3/2}$		
DOPANT DENSITY		$10^{13} < N_d < 2 \times 10^{16} \text{ cm}^{-3}$	$2 \times 10^{16} < N_d < 2 \times 10^{17} \text{ cm}^{-3}$	$2 \times 10^{17} < N_d < 10^{19} \text{ cm}^{-3}$
LATTICE MOBILITY	μ_L	μ_L values tabulated in ref. 1 table 1.	$\mu_L'' = R(Nd)\mu_L$ $R(Nd) = (1.013 \text{ to } 6.62) \times 10^{-19} \times Nd$	$\mu_L' = 0.88 \mu_L$
IONIZED IMPURITY MOBILITY	μ_I	$\mu_I = \frac{7.3 \times 10^{17} T^{3/2}}{N_I G(b_g)}$ $G(b_g) = 2n(b_g + 1) - \frac{b_g}{b_g + 1}$ $b_g = \frac{1.52 \times 10^{15} T^2}{n(2 - n/N_d)}$	$\mu_I'' = S(Nd)\mu_I$ $S(Nd) = (1.04 \text{ to } 2.04) \times 10^{-18} \times Nd$	$\mu_I' = 0.632 \mu_I$
MIXED SCATTERING FORMULA	μ_{LI}	$\mu_{LI} = \mu_L f(X)$ $f(X) = 1 + X^2(Ci(X)\cos X + \sin X(Si(X) - \pi/2))$ $X^2 = 6\mu_I/\mu_L$	$\mu_{LI}'' = \mu_L'' f(X'')$ $(X'')^2 = 6 \frac{\mu_L''}{\mu_I''}$	$\mu_{LI}' = \mu_L' f(X')$ $(X')^2 = 6 \frac{\mu_L'}{\mu_I'}$
NEUTRAL IMPURITY MOBILITY	μ_N	$\mu_N = \left(\frac{3 \times 10^{20}}{N_N} \right) \times (0.1495T^{1/2} + 1.482T^{-1/2})$	SAME	SAME
TOTAL ELECTRON MOBILITY	μ_n	$\mu_n = \left(\frac{1}{\mu_{LI}} + \frac{1}{\mu_N} \right)^{-1}$	$\mu_n = \left(\frac{1}{\mu_{LI}''} + \frac{1}{\mu_N} \right)^{-1}$	$\mu_n = \left(\frac{1}{\mu_{LI}'} + \frac{1}{\mu_N} \right)^{-1}$

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